Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:55 PM BST

PDB ID	:	4JZW
Title	:	Crystal structure of CD4-mimetic miniprotein M48U1 in complex with HIV-1 YU2 gp120 in P212121 space group
Authors	:	Acharya, P.; Kwong, P.D.
Deposited on	:	2013-04-03
Resolution	:	1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

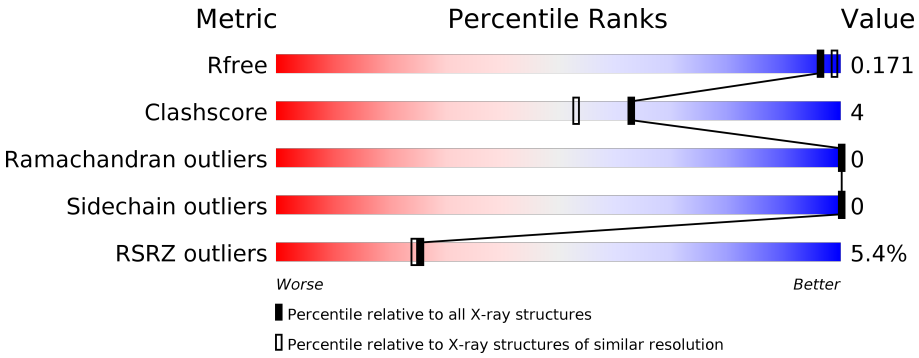
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	4% 83% 6% 11%
1	G	376	5% 82% 8% 10%
2	M	28	11% 93% 7%
2	R	28	14% 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	501	-	-	-	X
3	NAG	G	507	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7061 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

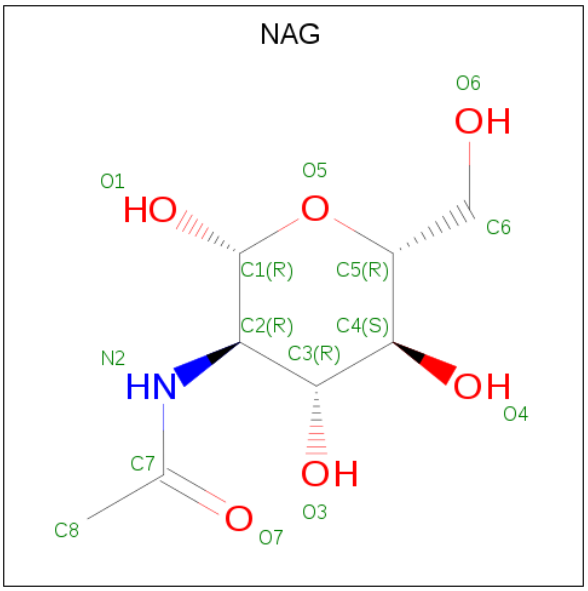
- Molecule 1 is a protein called HIV-1 YU2 gp120 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	14	0
			2678	1681	466	511	20			
1	G	339	Total	C	N	O	S	1	21	0
			2718	1702	467	524	25			

- Molecule 2 is a protein called CD4-MIMETIC MINIPROTEIN M48U1.

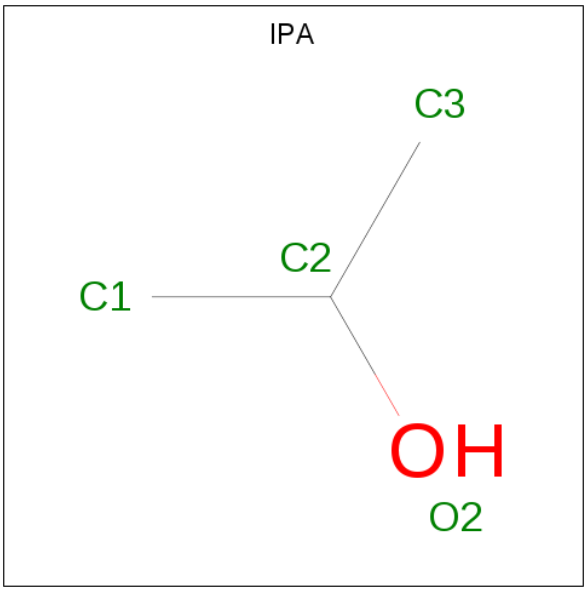
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	R	28	Total	C	N	O	S	0	3	1
			222	144	39	33	6			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



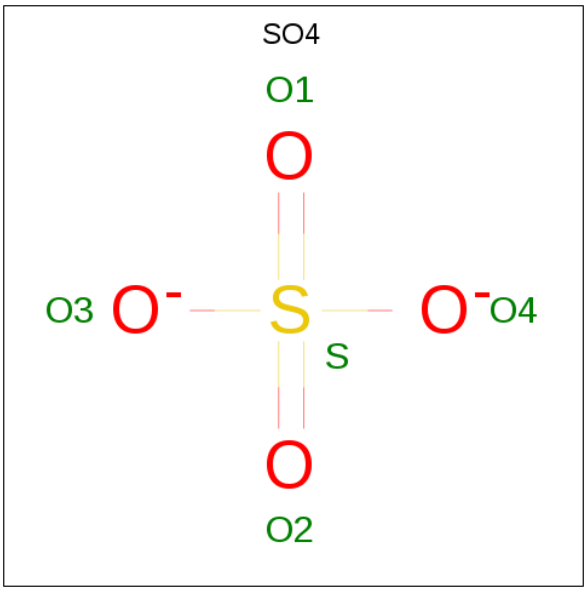
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



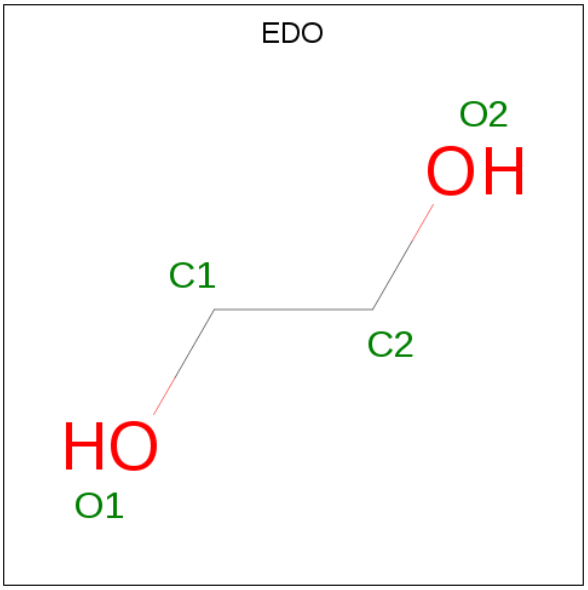
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 4 3 1	0	0
4	G	1	Total C O 4 3 1	0	0
4	G	1	Total C O 4 3 1	0	0
4	G	1	Total C O 4 3 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

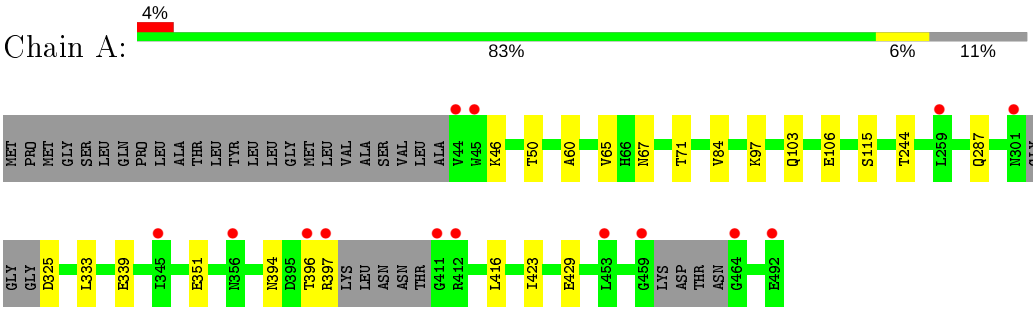
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	450	Total O 450 450	0	0
7	G	441	Total O 441 441	0	0
7	M	22	Total O 22 22	0	0
7	R	23	Total O 23 23	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

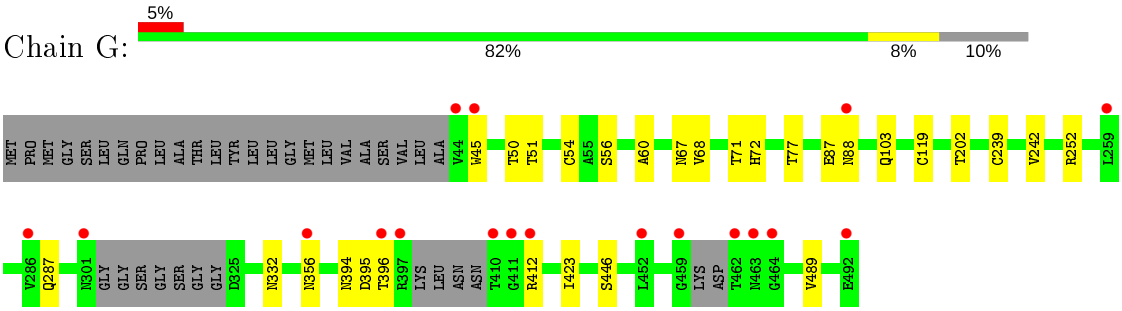
- Molecule 1: HIV-1 YU2 gp120 glycoprotein

Chain A:



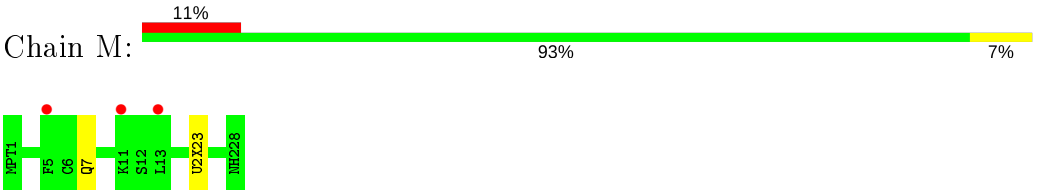
- Molecule 1: HIV-1 YU2 gp120 glycoprotein

Chain G:



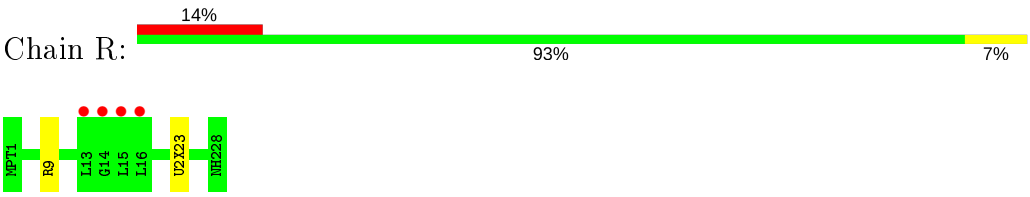
- Molecule 2: CD4-MIMETIC MINIPROTEIN M48U1

Chain M:



- Molecule 2: CD4-MIMETIC MINIPROTEIN M48U1

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.65Å 78.01Å 163.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.66 – 1.78 24.66 – 1.78	Depositor EDS
% Data completeness (in resolution range)	82.7 (24.66-1.78) 77.6 (24.66-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_755)	Depositor
R, R_{free}	0.164 , 0.209 0.175 , 0.171	Depositor DCC
R_{free} test set	3267 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7061	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5100e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, DPR, EDO, MPT, SO4, NH2, U2X, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/2797	0.56	0/3796
1	G	0.43	0/2879	0.56	0/3908
2	M	0.38	0/176	0.63	0/231
2	R	0.42	0/199	0.50	0/261
All	All	0.43	0/6051	0.56	0/8196

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2678	0	2611	19	0
1	G	2718	0	2643	25	0
2	M	209	0	212	1	0
2	R	222	0	237	1	0
3	A	140	0	130	5	0
3	G	112	0	104	2	0
4	A	20	0	40	1	0
4	G	12	0	24	2	0
5	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	5	0	0	1	0
6	G	4	0	6	0	0
7	A	450	0	0	11	0
7	G	441	0	0	10	0
7	M	22	0	0	1	0
7	R	23	0	0	0	0
All	All	7061	0	6007	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:NAG:H3	3:A:503:NAG:H83	1.59	0.84
1:G:54:CYS:O	7:G:1023:HOH:O	2.04	0.74
1:A:106[A]:GLU:OE2	7:A:851:HOH:O	2.04	0.73
1:A:351:GLU:OE1	7:A:860:HOH:O	2.06	0.72
1:A:394:ASN:O	7:A:928:HOH:O	2.12	0.68
4:A:516:IPA:H12	2:R:9:ARG:HE	1.60	0.66
1:G:356[A]:ASN:ND2	7:G:910:HOH:O	2.29	0.65
1:A:429:GLU:OE1	7:A:991:HOH:O	2.15	0.65
1:G:252:ARG:NH1	7:G:681:HOH:O	2.32	0.61
1:G:412:ARG:NH1	7:G:981:HOH:O	2.34	0.60
1:G:119:CYS:O	1:G:202[A]:THR:HG23	2.06	0.56
1:G:423:ILE:N	5:G:513:SO4:O2	2.39	0.55
3:A:503:NAG:H3	3:A:503:NAG:C8	2.33	0.55
1:G:394:ASN:ND2	3:G:507:NAG:O7	2.38	0.55
1:G:45:TRP:HB2	1:G:489[B]:VAL:CG1	2.36	0.55
1:A:325:ASP:N	7:A:918:HOH:O	2.39	0.55
2:M:7:GLN:OE1	7:M:204:HOH:O	2.19	0.53
1:A:97:LYS:NZ	7:A:1004:HOH:O	2.42	0.53
3:A:503:NAG:H2	7:A:997:HOH:O	2.10	0.52
1:G:446:SER:O	4:G:511:IPA:H31	2.10	0.51
1:A:71[A]:THR:HG22	7:A:715:HOH:O	2.08	0.51
1:G:45:TRP:HB2	1:G:489[B]:VAL:HG11	1.89	0.51
1:G:50:THR:O	1:G:103:GLN:NE2	2.38	0.50
3:A:503:NAG:H82	3:A:503:NAG:C1	2.41	0.50
1:G:71[A]:THR:HG22	7:G:660:HOH:O	2.12	0.50
1:A:46:LYS:NZ	7:A:1046:HOH:O	2.43	0.49
1:A:423:ILE:N	5:A:513:SO4:O2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:ALA:HA	1:G:71[A]:THR:HG21	1.95	0.48
1:A:60:ALA:HA	1:A:71[A]:THR:HG21	1.95	0.47
1:A:287:GLN:NE2	7:A:759:HOH:O	2.41	0.47
3:G:508:NAG:HN2	4:G:511:IPA:H11	1.81	0.46
1:G:87[A]:GLU:OE2	7:G:986:HOH:O	2.21	0.46
1:G:68:VAL:O	1:G:71[A]:THR:OG1	2.30	0.46
1:A:396:THR:O	1:A:397:ARG:HB3	2.16	0.46
1:G:287:GLN:NE2	7:G:715:HOH:O	2.47	0.46
1:G:72:HIS:ND1	7:G:1003:HOH:O	2.34	0.45
1:G:88:ASN:ND2	7:G:934:HOH:O	2.49	0.44
1:G:239[A]:CYS:SG	1:G:242:VAL:HG22	2.58	0.44
1:G:332:ASN:ND2	7:G:919:HOH:O	2.51	0.44
1:A:333:LEU:CD2	1:A:416[A]:LEU:HD11	2.48	0.44
1:G:50:THR:OG1	1:G:51:THR:N	2.51	0.43
1:G:67:ASN:O	1:G:71[A]:THR:HG23	2.18	0.43
1:A:50:THR:O	1:A:103:GLN:NE2	2.41	0.43
1:A:67:ASN:O	1:A:71[A]:THR:HG23	2.19	0.42
1:A:339:GLU:OE2	7:A:977:HOH:O	2.22	0.42
1:G:45:TRP:CD1	1:G:489[B]:VAL:HG11	2.55	0.41
1:A:65:VAL:HB	1:A:115:SER:HB3	2.02	0.41
1:G:56:SER:C	1:G:77[B]:THR:HG23	2.41	0.40
1:A:84:VAL:HB	1:A:244[A]:THR:CG2	2.51	0.40
1:G:395:ASP:OD1	1:G:396:THR:N	2.55	0.40
3:A:503:NAG:C1	3:A:503:NAG:C8	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/376 (91%)	335 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	353/376 (94%)	343 (97%)	10 (3%)	0	100	100
2	M	24/28 (86%)	23 (96%)	1 (4%)	0	100	100
2	R	27/28 (96%)	27 (100%)	0	0	100	100
All	All	745/808 (92%)	728 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/328 (94%)	310 (100%)	0	100	100
1	G	322/328 (98%)	322 (100%)	0	100	100
2	M	20/20 (100%)	20 (100%)	0	100	100
2	R	23/20 (115%)	23 (100%)	0	100	100
All	All	675/696 (97%)	675 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	U2X	M	23	2	19,20,21	1.61	3 (15%)	22,25,27	1.11	2 (9%)
2	U2X	R	23	2	19,20,21	1.57	3 (15%)	22,25,27	1.23	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	U2X	M	23	2	-	2/10/19/21	0/2/2/2
2	U2X	R	23	2	-	2/10/19/21	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	23	U2X	CE2-CD2	4.20	1.46	1.38
2	R	23	U2X	CE2-CD2	3.63	1.45	1.38
2	R	23	U2X	CE1-CD1	3.57	1.45	1.38
2	M	23	U2X	CE1-CD1	3.41	1.45	1.38
2	M	23	U2X	CB-CA	-2.57	1.48	1.53
2	R	23	U2X	CB-CA	-2.32	1.48	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	23	U2X	CB-CA-C	-2.81	106.20	111.47
2	R	23	U2X	OH-C7-C3	2.64	115.11	108.21
2	M	23	U2X	OH-C7-C3	2.38	114.42	108.21
2	R	23	U2X	C1-C2-C3	-2.37	107.67	112.15
2	M	23	U2X	CB-CA-C	-2.16	107.42	111.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	R	23	U2X	CE1-CZ-OH-C7

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Mol	Chain	Res	Type	Atoms
2	R	23	U2X	CE2-CZ-OH-C7
2	M	23	U2X	CE1-CZ-OH-C7
2	M	23	U2X	CE2-CZ-OH-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	G	508	1	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	A	508	1	14,14,15	0.27	0	17,19,21	0.46	0
4	IPA	A	512	-	3,3,3	0.58	0	3,3,3	0.29	0
3	NAG	A	504	1	14,14,15	0.31	0	17,19,21	0.35	0
5	SO4	A	513	-	4,4,4	0.20	0	6,6,6	0.23	0
3	NAG	A	506	1	14,14,15	0.20	0	17,19,21	0.36	0
5	SO4	G	513	-	4,4,4	0.22	0	6,6,6	0.26	0
3	NAG	A	514	1	14,14,15	0.23	0	17,19,21	0.38	0
3	NAG	G	503	1	14,14,15	0.46	0	17,19,21	0.39	0
4	IPA	A	511	-	3,3,3	0.60	0	3,3,3	0.22	0
4	IPA	G	509	-	3,3,3	0.56	0	3,3,3	0.19	0
3	NAG	G	507	1	14,14,15	0.43	0	17,19,21	0.41	0
4	IPA	G	511	-	3,3,3	0.59	0	3,3,3	0.20	0
3	NAG	A	507	1	14,14,15	0.39	0	17,19,21	0.47	0
3	NAG	A	509	1	14,14,15	0.28	0	17,19,21	0.39	0
4	IPA	G	510	-	3,3,3	0.57	0	3,3,3	0.19	0
3	NAG	A	505	1	14,14,15	0.51	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	G	502	1	14,14,15	0.30	0	17,19,21	0.51	0
4	IPA	A	510	-	3,3,3	0.55	0	3,3,3	0.17	0
3	NAG	G	506	1	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	G	501	1	14,14,15	0.30	0	17,19,21	0.42	0
3	NAG	A	502	1	14,14,15	0.54	0	17,19,21	0.40	0
3	NAG	A	503	1	14,14,15	0.29	0	17,19,21	0.72	0
4	IPA	A	515	-	3,3,3	0.57	0	3,3,3	0.20	0
6	EDO	G	512	-	3,3,3	0.45	0	2,2,2	0.28	0
3	NAG	G	504	1	14,14,15	0.29	0	17,19,21	0.38	0
3	NAG	G	505	1	14,14,15	0.30	0	17,19,21	0.44	0
3	NAG	A	501	1	14,14,15	0.80	1 (7%)	17,19,21	0.69	1 (5%)
4	IPA	A	516	-	3,3,3	0.59	0	3,3,3	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	508	1	-	0/6/23/26	0/1/1/1
3	NAG	G	503	1	-	0/6/23/26	0/1/1/1
3	NAG	A	508	1	-	0/6/23/26	0/1/1/1
3	NAG	G	507	1	-	4/6/23/26	0/1/1/1
3	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	EDO	G	512	-	-	1/1/1/1	-
3	NAG	A	514	1	-	0/6/23/26	0/1/1/1
3	NAG	A	507	1	-	2/6/23/26	0/1/1/1
3	NAG	G	504	1	-	3/6/23/26	0/1/1/1
3	NAG	A	509	1	-	0/6/23/26	0/1/1/1
3	NAG	G	505	1	-	1/6/23/26	0/1/1/1
3	NAG	A	505	1	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	G	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	G	506	1	-	0/6/23/26	0/1/1/1
3	NAG	G	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	C1-C2	2.48	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	NAG	C1-O5-C5	2.18	115.15	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	507	NAG	C3-C2-N2-C7
3	G	507	NAG	O5-C5-C6-O6
3	G	504	NAG	O5-C5-C6-O6
3	G	507	NAG	C4-C5-C6-O6
3	G	504	NAG	C4-C5-C6-O6
3	A	503	NAG	C8-C7-N2-C2
3	A	503	NAG	O7-C7-N2-C2
3	A	507	NAG	O5-C5-C6-O6
3	A	503	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
6	G	512	EDO	O1-C1-C2-O2
3	A	507	NAG	C4-C5-C6-O6
3	A	503	NAG	C3-C2-N2-C7
3	G	505	NAG	O5-C5-C6-O6
3	G	507	NAG	C1-C2-N2-C7
3	G	504	NAG	C1-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	508	NAG	1	0
5	A	513	SO4	1	0
5	G	513	SO4	1	0
3	G	507	NAG	1	0
4	G	511	IPA	2	0
3	A	503	NAG	5	0
4	A	516	IPA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	336/376 (89%)	-0.08	14 (4%)	36	34	22, 31, 58, 110	0
1	G	339/376 (90%)	0.01	18 (5%)	26	25	22, 31, 59, 110	0
2	M	24/28 (85%)	0.33	3 (12%)	3	3	27, 52, 73, 84	0
2	R	24/28 (85%)	0.31	4 (16%)	1	1	25, 46, 60, 61	0
All	All	723/808 (89%)	-0.01	39 (5%)	25	24	22, 32, 60, 110	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	410	THR	8.4
1	G	462	THR	6.8
1	G	397	ARG	6.3
1	A	397	ARG	6.3
1	G	44	VAL	5.9
1	G	463	ASN	5.1
1	G	356[A]	ASN	5.0
1	G	45	TRP	4.5
1	A	464	GLY	3.9
2	R	14	GLY	3.9
1	A	459	GLY	3.6
1	A	356	ASN	3.6
1	A	396	THR	3.4
1	A	301	ASN	3.4
1	G	411	GLY	3.3
1	A	44	VAL	3.3
1	G	464	GLY	3.1
1	A	45	TRP	3.0
2	M	5	PHE	3.0
1	G	396	THR	2.9
1	G	452	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	R	15	LEU	2.8
1	A	412	ARG	2.7
1	G	88	ASN	2.7
1	G	259	LEU	2.7
1	A	492	GLU	2.6
1	G	301	ASN	2.5
2	R	13	LEU	2.5
1	A	345	ILE	2.4
1	A	259	LEU	2.4
1	G	286	VAL	2.3
1	G	492	GLU	2.2
1	G	459	GLY	2.2
1	G	412	ARG	2.2
2	R	16[A]	LEU	2.1
1	A	411	GLY	2.1
2	M	11	LYS	2.0
1	A	453	LEU	2.0
2	M	13	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	U2X	R	23	19/20	0.94	0.10	21,25,34,36	0
2	U2X	M	23	19/20	0.97	0.08	22,26,32,34	0
2	DPR	M	21	7/8	0.98	0.06	25,26,28,29	0
2	DPR	R	21	7/8	0.98	0.04	22,25,26,27	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	501	14/15	0.53	0.67	118,126,131,132	0
3	NAG	G	507	14/15	0.75	0.43	102,119,122,126	0
3	NAG	G	504	14/15	0.80	0.26	57,66,82,90	0
3	NAG	A	506	14/15	0.81	0.22	51,60,79,90	0
4	IPA	A	515	4/4	0.84	0.38	80,80,82,84	0
4	IPA	A	516	4/4	0.87	0.32	68,71,73,74	0
4	IPA	G	511	4/4	0.88	0.21	62,63,69,79	0
3	NAG	A	503	14/15	0.88	0.15	59,67,74,74	0
3	NAG	A	509	14/15	0.89	0.28	49,58,65,67	0
3	NAG	A	504	14/15	0.89	0.19	50,58,63,69	0
3	NAG	G	501	14/15	0.90	0.20	49,56,66,67	0
3	NAG	A	514	14/15	0.90	0.15	59,65,68,69	0
3	NAG	G	508	14/15	0.91	0.30	45,57,72,76	0
4	IPA	A	511	4/4	0.91	0.12	46,51,52,54	0
6	EDO	G	512	4/4	0.91	0.28	62,62,64,65	0
3	NAG	G	506	14/15	0.93	0.13	35,48,60,69	0
4	IPA	G	509	4/4	0.93	0.13	32,36,39,46	0
3	NAG	A	507	14/15	0.93	0.15	48,58,68,72	0
3	NAG	A	508	14/15	0.93	0.18	40,61,68,71	0
3	NAG	G	505	14/15	0.94	0.14	49,53,71,75	0
4	IPA	A	512	4/4	0.94	0.19	41,46,46,47	0
3	NAG	G	502	14/15	0.94	0.09	29,35,44,45	0
4	IPA	G	510	4/4	0.95	0.09	36,42,44,47	0
5	SO4	A	513	5/5	0.96	0.18	26,32,35,55	5
3	NAG	G	503	14/15	0.96	0.07	29,33,45,46	0
4	IPA	A	510	4/4	0.96	0.11	37,41,41,49	0
3	NAG	A	505	14/15	0.97	0.07	27,30,42,46	0
3	NAG	A	502	14/15	0.97	0.06	30,33,47,53	0
5	SO4	G	513	5/5	0.97	0.14	26,30,31,45	5

6.5 Other polymers (i)

There are no such residues in this entry.